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STRUCTURE FILE UPDATES: 24 APR 2007 HIGHEST RN 932392-31-9  
DICTIONARY FILE UPDATES: 24 APR 2007 HIGHEST RN 932392-31-9

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=>  
Uploading C:\Program Files\Stnexp\Queries\10573204.str



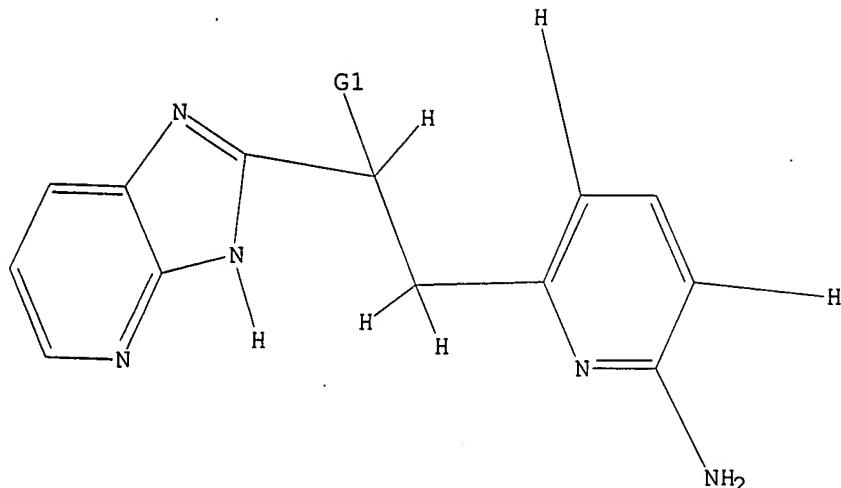
chain nodes :  
 10 11 18 19 20 21 22 23 24 27  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 12 13 14 15 16 17  
 chain bonds :  
 8-10 9-19 10-11 10-20 10-27 11-12 11-21 11-22 13-23 15-24 16-18  
 ring bonds :  
 1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9 12-13 12-17 13-14 14-15 15-16  
 16-17  
 exact/norm bonds :  
 3-7 4-9 7-8 8-9 10-27 16-18  
 exact bonds :  
 8-10 9-19 10-11 10-20 11-12 11-21 11-22 13-23 15-24  
 normalized bonds :  
 1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17  
 isolated ring systems :  
 containing 1 : 12 :

G1:C,H

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS  
 11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS  
 20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 27:CLASS

L1 STRUCTURE UPLOADED

=> d 11  
L1 HAS NO ANSWERS  
L1 STR



G1 C, H

Structure attributes must be viewed using STN Express query preparation.

=> s 11  
SAMPLE SEARCH INITIATED 12:54:26 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 8 TO 329  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full  
FULL SEARCH INITIATED 12:54:30 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 163 TO ITERATE

100.0% PROCESSED 163 ITERATIONS 27 ANSWERS  
SEARCH TIME: 00.00.01

L3 27 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
FULL ESTIMATED COST ENTRY SESSION  
172.10 172.31

FILE 'CAPLUS' ENTERED AT 12:54:35 ON 25 APR 2007  
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FILE COVERS 1907 - 25 Apr 2007 VOL 146 ISS 18  
FILE LAST UPDATED: 24 Apr 2007 (20070424/ED)

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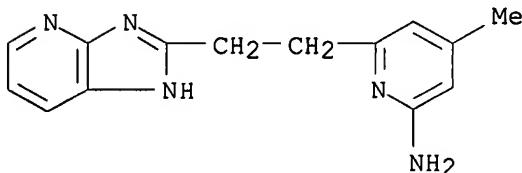
=> s 13 full  
L4 2 L3

=> d ibib abs hitstr tot

L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2006:43156 CAPLUS  
DOCUMENT NUMBER: 144:163527  
TITLE: The novel imidazopyridine 2-[2-(4-Methoxy-pyridin-2-yl)-ethyl]-3H-imidazo[4,5-b]pyridine (BYK191023) is a highly selective inhibitor of the inducible nitric-oxide synthase  
AUTHOR(S): Strub, Andreas; Ulrich, Wolf-Ruediger; Hesslinger, Christian; Eltze, Manfrid; Fuchss, Thomas; Strassner, Jochen; Strand, Susanne; Lehner, Martin D.; Boer, Rainer  
CORPORATE SOURCE: Departments of Biochemistry, Chemistry and Pharmacology, ALTANA Pharma AG, Konstanz, Germany  
SOURCE: Molecular Pharmacology (2006), 69(1), 328-337  
CODEN: MOPMA3; ISSN: 0026-895X  
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB We have identified imidazopyridine derivs. as a novel class of NO synthase inhibitors with high selectivity for the inducible isoform. 2-[2-(4-Methoxy-pyridin-2-yl)-ethyl]-3H-imidazo[4,5-b]pyridine (BYK191023) showed half-maximal inhibition of crudely purified human inducible (iNOS), neuronal (nNOS), and endothelial (eNOS) NO synthases at 86 nM, 17  $\mu$ M, and 162  $\mu$ M, resp. Inhibition of inducible NO synthase was competitive with L-arginine, pointing to an interaction of BYK191023 with the catalytic center of the enzyme. In radioligand and surface plasmon resonance expts., BYK191023 exhibited an affinity for iNOS, nNOS, and eNOS of 450 nM, 30  $\mu$ M, and >500  $\mu$ M, resp. Inhibition of cellular nitrate/nitrite synthesis in RAW, rat mesangium, and human embryonic kidney 293 cells after iNOS induction showed 40- to 100-fold higher IC50 values than at the isolated enzyme, in agreement with the much higher L-arginine concns. in cell culture media and inside intact cells. BYK191023 did not show any toxicity in various rodent and human cell lines up to high micromolar concns. The inhibitory potency of BYK191023 was tested in isolated organ models of iNOS (lipopolysaccharide-treated and phenylephrine-precontracted rat aorta; IC50 = 7  $\mu$ M), eNOS (arecaidine propargyl ester-induced relaxation of phenylephrine-precontracted rat aorta; IC50 > 100  $\mu$ M), and nNOS (field-stimulated relaxation of phenylephrine-precontracted rabbit corpus cavernosum; IC50 > 100  $\mu$ M). These data confirm the high selectivity of BYK191023 for iNOS over eNOS and nNOS found at isolated enzymes. In summary, we have identified a new

highly selective iNOS inhibitor structurally unrelated to known compds. and L-arginine. BYK191023 is a valuable tool for the investigation of iNOS-mediated effects in vitro and in vivo.

IT 857379-46-5, BYK 237007  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (structure activity relationship studied of imidazopyridine compds. as selective inhibitors of nitric-oxide synthase isoforms)  
 RN 857379-46-5 CAPLUS  
 CN 2-Pyridinamine, 6-[2-(1H-imidazo[4,5-b]pyridin-2-yl)ethyl]-4-methyl- (9CI)  
 (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2005:588961 CAPLUS  
 DOCUMENT NUMBER: 143:115536  
 TITLE: A preparation of (aminopyridinylethyl)imidazolopyridine derivatives, useful as inductible NO-synthase inhibitors  
 INVENTOR(S): Boer, Rainer; Marx, Degenhard; Ulrich, Wolf-Ruediger; Eltze, Manfrid; Nave, Ruediger; Strub, Andreas; Graedler, Ulrich; Fuchss, Thomas  
 PATENT ASSIGNEE(S): Altana Pharma A.-G., Germany  
 SOURCE: PCT Int. Appl., 63 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

| PATENT NO.   | KIND | DATE     | APPLICATION NO.  | DATE     |
|--|------|----------|------------------|----------|
| WO 2005061496  | A1   | 20050707 | WO 2004-EP52373  | 20040930 |
| WO 2005061496  | A8   | 20060216 |                  |          |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,<br>CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,<br>GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,<br>LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,<br>NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,<br>TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW |      |          |                  |          |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,<br>AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,<br>EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,<br>SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,<br>SN, TD, TG   |      |          |                  |          |
| AU 2004303515  | A1   | 20050707 | AU 2004-303515   | 20040930 |
| CA 2540230   | A1   | 20050707 | CA 2004-2540230  | 20040930 |
| EP 1670798   | A1   | 20060621 | EP 2004-820599   | 20040930 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,<br>IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR   |      |          |                  |          |
| CN 1856493   | A    | 20061101 | CN 2004-80027807 | 20040930 |
| BR 2004015034  | A    | 20061212 | BR 2004-15034    | 20040930 |
| JP 2007507464  | T    | 20070329 | JP 2006-530261   | 20040930 |
| US 2007043072  | A1   | 20070222 | US 2006-573204   | 20060324 |

NO 2006001789  
PRIORITY APPLN. INFO.:

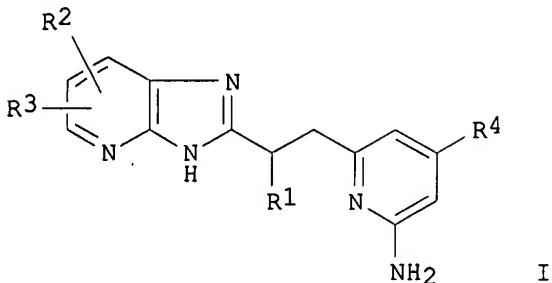
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NO 2006-1789  
EP 2003-22040  
WO 2004-EP52373

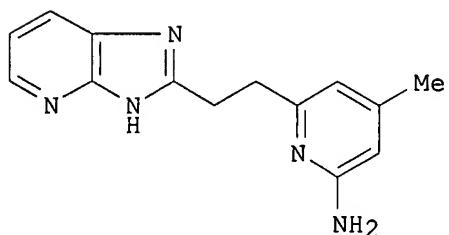
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A 20031001  
W 20040930

OTHER SOURCE(S):  
GI

MARPAT 143:115536



I



II

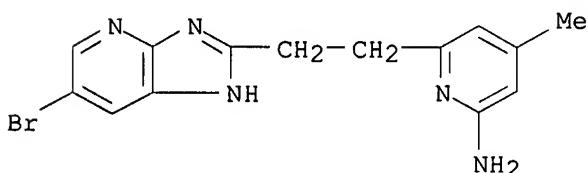
AB The invention relates to a preparation of (aminopyridinylethyl)imidazolopyridine derivs. of formula I [wherein: R1 is H or alkyl; R2 is H, halogen, NH2, (cyclo)alkyl, or CF3, etc.; R3 is H, halogen, alkyl, or alkoxy; R4 is alkyl or alkoxy], useful as antiinflammatory agents (inducible NO-synthase inhibitors). For instance, (aminopyridinylethyl)imidazolopyridine derivative II was prepared via condensation of 4-methyl-2-(tritylaminopicolinaldehyde with [3H-imidazo[4,5-b]pyridin-2-ylmethyl]triphenylphosphonium chloride and subsequent reduction of the obtained intermediate. The invention compds. were tested for NO-synthase activity [-log IC50(mol/L) values range from 6.58 to 8.15].

IT 857379-53-4P 857379-56-7P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of (aminopyridinylethyl)imidazolopyridine derivs. useful as inducible NO-synthase inhibitors)

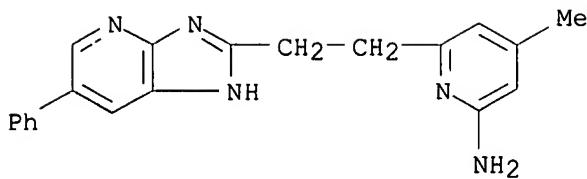
RN 857379-53-4 CAPLUS

CN 2-Pyridinamine, 6-[2-(6-bromo-1H-imidazo[4,5-b]pyridin-2-yl)ethyl]-4-methyl- (9CI) (CA INDEX NAME)



RN 857379-56-7 CAPLUS

CN 2-Pyridinamine, 4-methyl-6-[2-(6-phenyl-1H-imidazo[4,5-b]pyridin-2-yl)ethyl]- (9CI) (CA INDEX NAME)



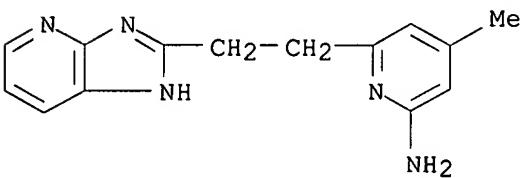
IT 857379-46-5P 857379-49-8P 857379-50-1P  
 857379-51-2P 857379-57-8P 857379-58-9P  
 857379-61-4P 857379-63-6P 857379-65-8P  
 857379-66-9P 857379-68-1P 857379-69-2P  
 857379-71-6P 857379-72-7P 857379-73-8P  
 857379-74-9P 857379-75-0P 857379-76-1P  
 857379-77-2P 857379-78-3P 857379-79-4P  
 857379-81-8P 857380-22-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (aminopyridinylethyl)imidazolopyridine derivs. useful as inductive NO-synthase inhibitors)

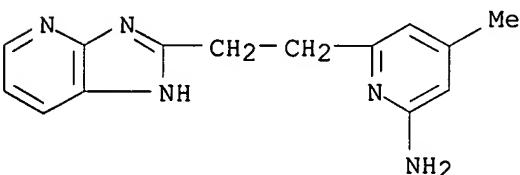
RN 857379-46-5 CAPLUS

CN 2-Pyridinamine, 6-[2-(1H-imidazo[4,5-b]pyridin-2-yl)ethyl]-4-methyl- (9CI)  
 (CA INDEX NAME)



RN 857379-49-8 CAPLUS

CN 2-Pyridinamine, 6-[2-(1H-imidazo[4,5-b]pyridin-2-yl)ethyl]-4-methyl-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

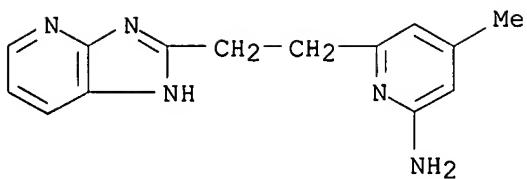
RN 857379-50-1 CAPLUS

CN 2-Pyridinamine, 6-[2-(1H-imidazo[4,5-b]pyridin-2-yl)ethyl]-4-methyl-, acetate (9CI) (CA INDEX NAME)

CM 1

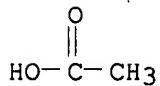
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CMF C14 H15 N5

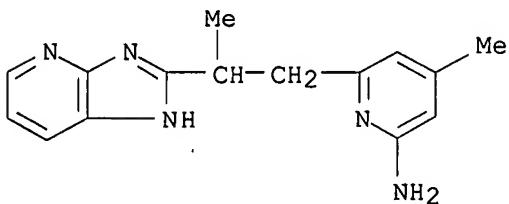


CM 2

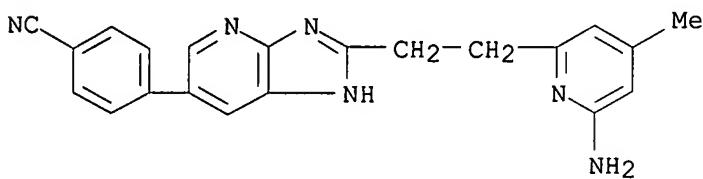
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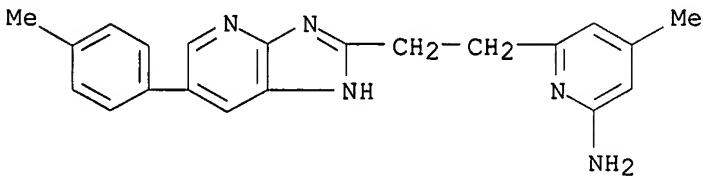
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CN 2-Pyridinamine, 6-[2-(1H-imidazo[4,5-b]pyridin-2-yl)propyl]-4-methyl- (9CI) (CA INDEX NAME)



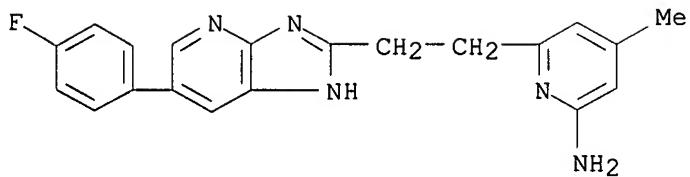
RN 857379-57-8 CAPLUS  
CN Benzonitrile, 4-[2-[2-(6-amino-4-methyl-2-pyridinyl)ethyl]-1H-imidazo[4,5-b]pyridin-6-yl]- (9CI) (CA INDEX NAME)



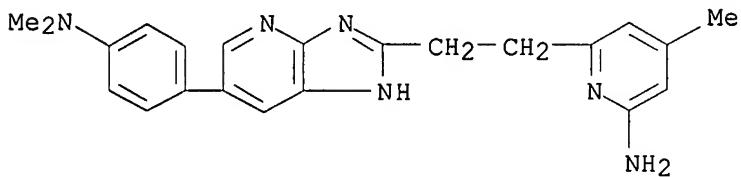
RN 857379-58-9 CAPLUS  
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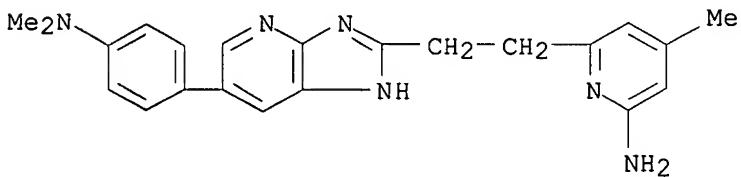
RN 857379-61-4 CAPLUS  
CN 2-Pyridinamine, 6-[2-[6-(4-fluorophenyl)-1H-imidazo[4,5-b]pyridin-2-yl]ethyl]-4-methyl- (9CI) (CA INDEX NAME)



RN 857379-63-6 CAPLUS  
 CN 2-Pyridinamine, 6-[2-[6-[4-(dimethylamino)phenyl]-1H-imidazo[4,5-b]pyridin-2-yl]ethyl]-4-methyl- (9CI) (CA INDEX NAME)

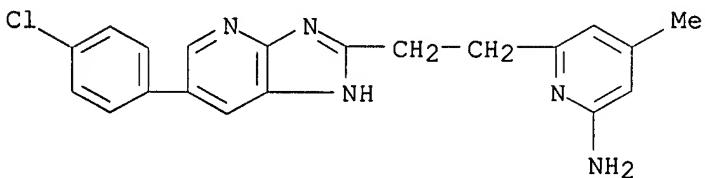


RN 857379-65-8 CAPLUS  
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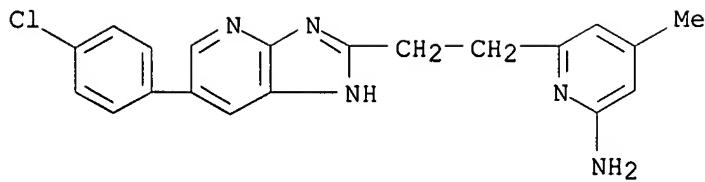


● HCl

RN 857379-66-9 CAPLUS  
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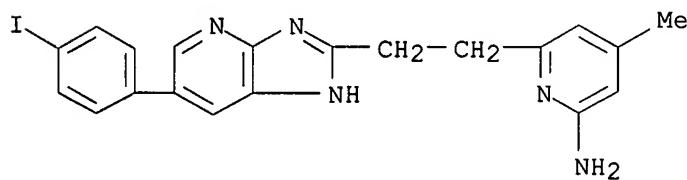


RN 857379-68-1 CAPLUS  
 CN 2-Pyridinamine, 6-[2-[6-(4-chlorophenyl)-1H-imidazo[4,5-b]pyridin-2-yl]ethyl]-4-methyl-, hydrochloride (9CI) (CA INDEX NAME)

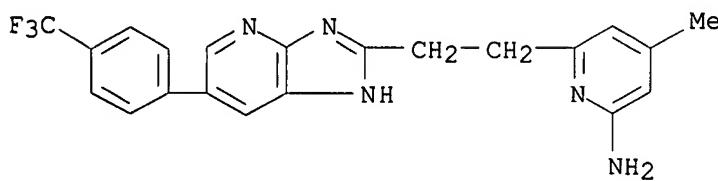


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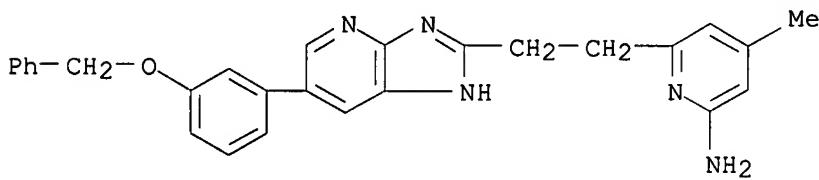
RN 857379-69-2 CAPLUS  
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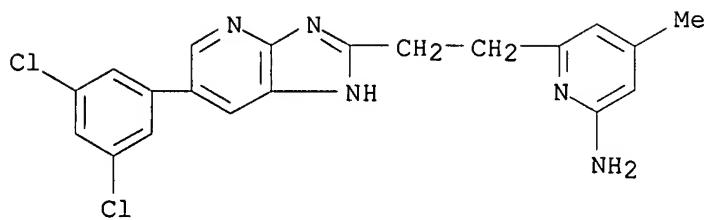
RN 857379-71-6 CAPLUS  
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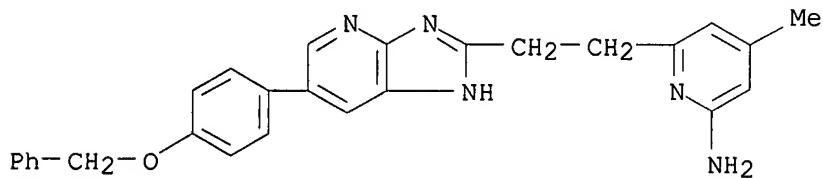
RN 857379-72-7 CAPLUS  
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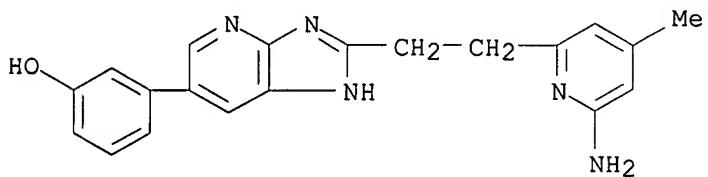
RN 857379-73-8 CAPLUS  
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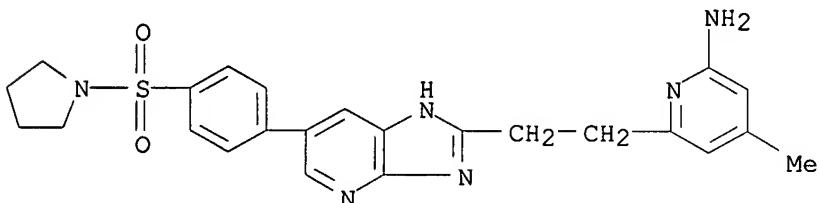
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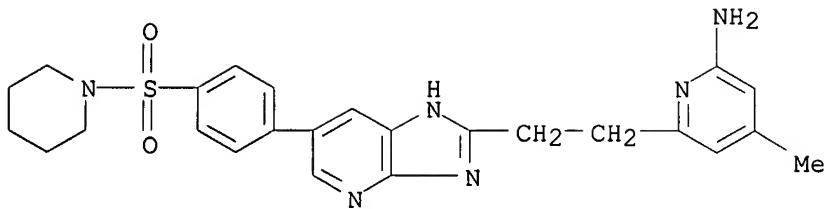
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 CN Phenol, 3-[2-[2-(6-amino-4-methyl-2-pyridinyl)ethyl]-1H-imidazo[4,5-b]pyridin-6-yl]- (9CI) (CA INDEX NAME)



RN 857379-76-1 CAPLUS  
 CN Pyrrolidine, 1-[[4-[2-[2-(6-amino-4-methyl-2-pyridinyl)ethyl]-1H-imidazo[4,5-b]pyridin-6-yl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)

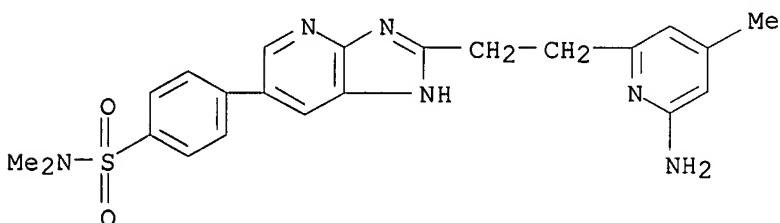


RN 857379-77-2 CAPLUS  
 CN Piperidine, 1-[[4-[2-[2-(6-amino-4-methyl-2-pyridinyl)ethyl]-1H-imidazo[4,5-b]pyridin-6-yl]phenyl]sulfonyl]- (9CI) (CA INDEX NAME)



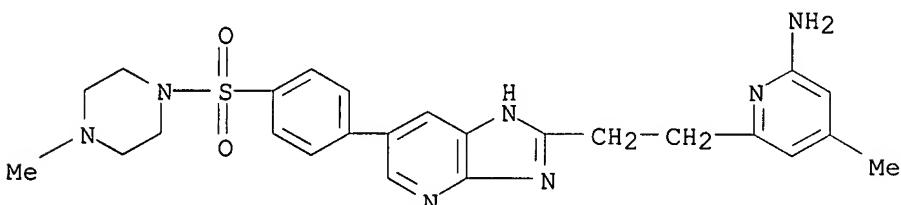
RN 857379-78-3 CAPLUS

CN Benzenesulfonamide, 4-[2-[2-(6-amino-4-methyl-2-pyridinyl)ethyl]-1H-imidazo[4,5-b]pyridin-6-yl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 857379-79-4 CAPLUS

CN Piperazine, 1-[[4-[2-[2-(6-amino-4-methyl-2-pyridinyl)ethyl]-1H-imidazo[4,5-b]pyridin-6-yl]phenyl]sulfonyl]-4-methyl- (9CI) (CA INDEX NAME)



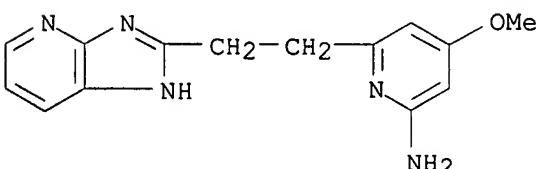
RN 857379-81-8 CAPLUS

CN 2-Pyridinamine, 6-[2-(1H-imidazo[4,5-b]pyridin-2-yl)ethyl]-4-methoxy-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 857379-80-7

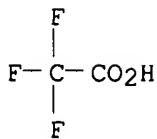
CMF C14 H15 N5 O



CM 2

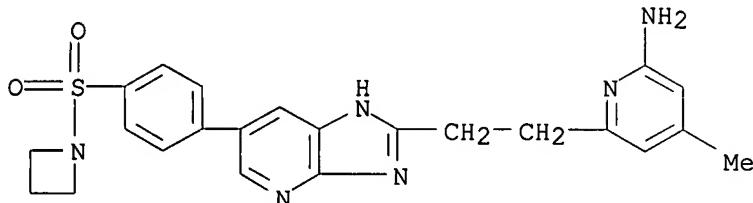
CRN 76-05-1

CMF C2 H F3 O2



RN 857380-22-4 CAPLUS

CN Azetidine, 1-[4-[2-[6-amino-4-methyl-2-pyridinyl]ethyl]-1H-imidazo[4,5-b]pyridin-6-yl]phenylsulfonyl]- (9CI) (CA INDEX NAME)

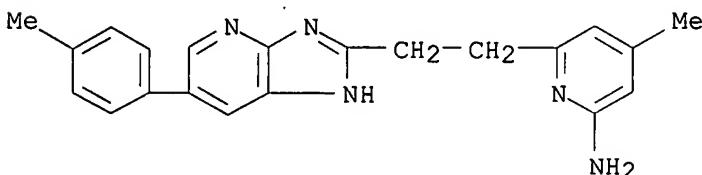


IT 857379-60-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of (aminopyridinylethyl)imidazolopyridine derivs. useful as inductive NO-synthase inhibitors)

RN 857379-60-3 CAPLUS

CN 2-Pyridinamine, 4-methyl-6-[2-[6-(4-methylphenyl)-1H-imidazo[4,5-b]pyridin-2-yl]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 12:53:39 ON 25 APR 2007)

FILE 'REGISTRY' ENTERED AT 12:53:49 ON 25 APR 2007  
STRUCTURE UPLOADED

L1 0 S L1  
L2 27 S L1 FULL  
L3 27 S L1 FULL

FILE 'CAPLUS' ENTERED AT 12:54:35 ON 25 APR 2007  
L4 2 S L3 FULL

=> log y  
COST IN U.S. DOLLARS

| SINCE FILE ENTRY | TOTAL SESSION |
|------------------|---------------|
|------------------|---------------|

|  |            |         |
|--|------------|---------|
| FULL ESTIMATED COST                        | 11.01      | 183.32  |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL   |
| CA SUBSCRIBER PRICE                        | ENTRY      | SESSION |
|  | -1.56      | -1.56   |

STN INTERNATIONAL LOGOFF AT 12:55:20 ON 25 APR 2007